[0042] Here, (e) is the elementary charge, (mu=1.6605×10^{-27} kg) is the atomic mass unit, ($\omega=2\pi f$) is the angular frequency, (h0≈0.5 mm) is the distance corresponding to the onset of ion losses on the surface of the ring electrodes, and (δ) is related to the distance between the ring electrodes, d=1 mm, as ($\delta=d/\pi$). Assuming that the trapped ion ensemble is limited to $(m/z)_{high}\approx2000$ amu, using (f)=600 kHz and the electric field characteristic for the dc trapping conditions, (E_n)=20 V/cm, from equation (1) the rf-voltage (V_{RF})≈30V, or 60 V_{p-p}, which is consistent with experimentally observed rf-amplitudes. In the continuous mode, both dc-trapping and space charge components of (E_n) are reduced, which provides different (V_{RF}) values. Trapping efficiency strongly depends on the axial dc-gradient, e.g., as shown by the dependence of Reserpine monoisotopic peak intensity (FIG. **8**) on the extraction time at four different dc-gradients in the trapping portion. Reduction of the dc gradient from 20 V/cm to 4 V/cm resulted in a more than 2 orders of magnitude improvement in sensitivity and an ion extraction time of 100 μs. Fast removal of ions from the IFT was important for efficient coupling of the ion trap to a subsequent ion stage, e.g., the oa-TOF mass spectrometer described herein. Ion current was measured at the collisional quadrupole and the charge collector (FIG. **5**) in both the trapping and continuous modes. Estimate of trapping efficiency can be made based on comparison of ion signals at the collisional quadrupole in continuous and trapping modes.

Example 4

SIMION 8.0 Simulations

Profiles of Effective and DC Potentials in Dual Exit Grid Configuration for Ion Accumulation and Ion Ejection

[0043] Ion accumulation and ejection from the IFT in both single- and dual-grid configurations were modeled using commercially available SIMION 8.0 software (Scientific Instrument Services, Ringoes, N.J.). Full potential distribution of the dual gate design was relatively uniform along the axis throughout the trapping portion of the IFT. A single gate configuration reduces overall trapping capacity of the IFT but also necessitates use of longer extraction times for full ion ejection. Specific spatial and electrical configurations of the two grids at the IFT exit enabled both effective ion accumulation and ejection. During an exemplary ejection event, potential of the trapping grid was ramped to ~50 V. Electric field gradient for the 5 mm ion trap segment immediately preceding the trapping grid was ~19 V/cm. A strong electric field at the IFT exit ensured fast ion ejection from the trap. The IFT was modeled using simulations performed with SIMION 8.0 (Scientific Instrument Services, Ringoes, N.J.) software that simulates motion of charged particles in rf-fields. Ion collisions with nitrogen buffer gas were modeled assuming ion-neutral hard-sphere collision using a code available with SIMION 8.0. A group of 50 particles with a total charge of 1.6×10^{-13} C (distributed equally on the particles) were flown through 1 Torr of static nitrogen buffer gas. As charged particles travel within the trap, they experience an oscillating rf-field in addition to dc-gradient. Charged particles were stored in the IFT by applying a trapping voltage to entrance grid. After trapping for 2 ms, voltage on the entrance grid was lowered to release the ions. Simulations were performed for singly charged Reserpine (m/z=609) at an rf-frequency of 600 kHz and an rf-amplitude of 74 V_{p-p} and for 20 V/cm and 4 V/cm dc-gradients in the IFT. Under 20 V/cm dc-gradient conditions, 36 particles were lost on electrodes before being released from the trap (72% loss). No particles were lost during trapping with a 4 V/cm dc-gradient. The effective potential (V*) was derived according to the following equation:

$$V*(r,z)=\frac{q^2E_{RF}^2(r,z)}{4m\omega^2}$$

[0044] Here, q=ze is the ion charge; $E_{RF}(r, z)$ is the amplitude of the rf-electric field; m is the ion mass, and ω is the angular frequency of the rf-field. The dc-gradient was superimposed on (V*) to generate a full effective potential. Calculated full effective potentials were normalized to the potential at the trap entrance for direct comparison. Under 20 V/cm dc-gradient, ions are trapped in a well of ~8 V very close to the trap exit electrode leading to their instability and loss. Under trap dc-gradient of 4 V/cm, effective potential shows no distinct region where ions can be directed into. Accordingly, accumulated ions are closer to the trap axis rather than near the electrodes.

CONCLUSIONS

[0045] An ion trap has been described that operates at pressures which enable seamless interfacing to atmospheric pressure ionization sources. The trap operating pressure can also be increased for, e.g., more efficient coupling to mobility separations. For example, in an exemplary configuration, the IFT is characterized by an extraction time of 40 μs for multiply charged ions and 100 μs for singly charged species. Performance of the IFT coupled to a TOF-MS was examined in both trapping and continuous modes. In the continuous mode, TOF MS provides a high pulsing rate of ~10 kHz, and given sufficient ion current, each successive TOF pulse can deliver ions to the detector. In trapping mode, only 100-1000 ion packets are delivered to the TOF detector over the same acquisition period. However, packets of ions accumulated in the IFT are characterized by higher charge density than those in continuous mode. Improved S/N in the trapping mode results from a combination of factors that contribute to an increase in signal intensity and a decrease in the chemical background. Ion accumulation in the trap appears to be particularly advantageous at very low analyte concentrations. Ion packets exiting the IFT are characterized by higher ion densities and, therefore, result in higher S/N values. In addition, the IFT facilitates more efficient desolvation of ions resulting in substantial reduction in background noise and further S/N improvement. Incorporation of a dual-grid gating design in the IFT increases effective charge capacity, ejection efficiency, and ion packet charge density. A 7-fold increase in signal is observed based on comparisons of a pulsed ion current obtained from IFT-IMS experiments against a continuous ion current. The IFT allows injection of ion packets with ion densities that are 1 order of magnitude greater than conventional IMS gating mechanisms. Additional comparisons between trapped and continuous signal levels indicate that, for minimal ion accumulation times, ion utilization efficiency of the IFT approaches 100%. While these short accumulation times (<10 ms) are much less than a typical IMS scan time (~60 ms), such accumulation times are an ideal length for integration with other approaches, including multiplexing, to enhance instrumental duty cycle. By combining